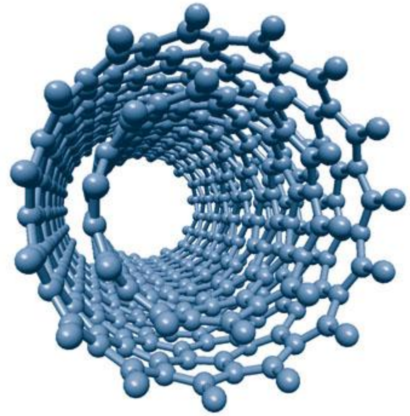
Modeling Tools for Environmental and Economic Uncertainties in Nanomanufacturing



Center for High-rate Nanomanufacturing

NSRG Nanotechnology & Society Research Group

QPL Quality & Productivity Laboratory

Northeastern University

Jacqueline A. Isaacs

Associate Director, Center for High-rate Nanomanufacturing

Professor, Mechanical and Industrial Engineering

Northeastern University, Boston MA

New England Nanomanufacturing Summit 2010

Lowell, Massachusetts

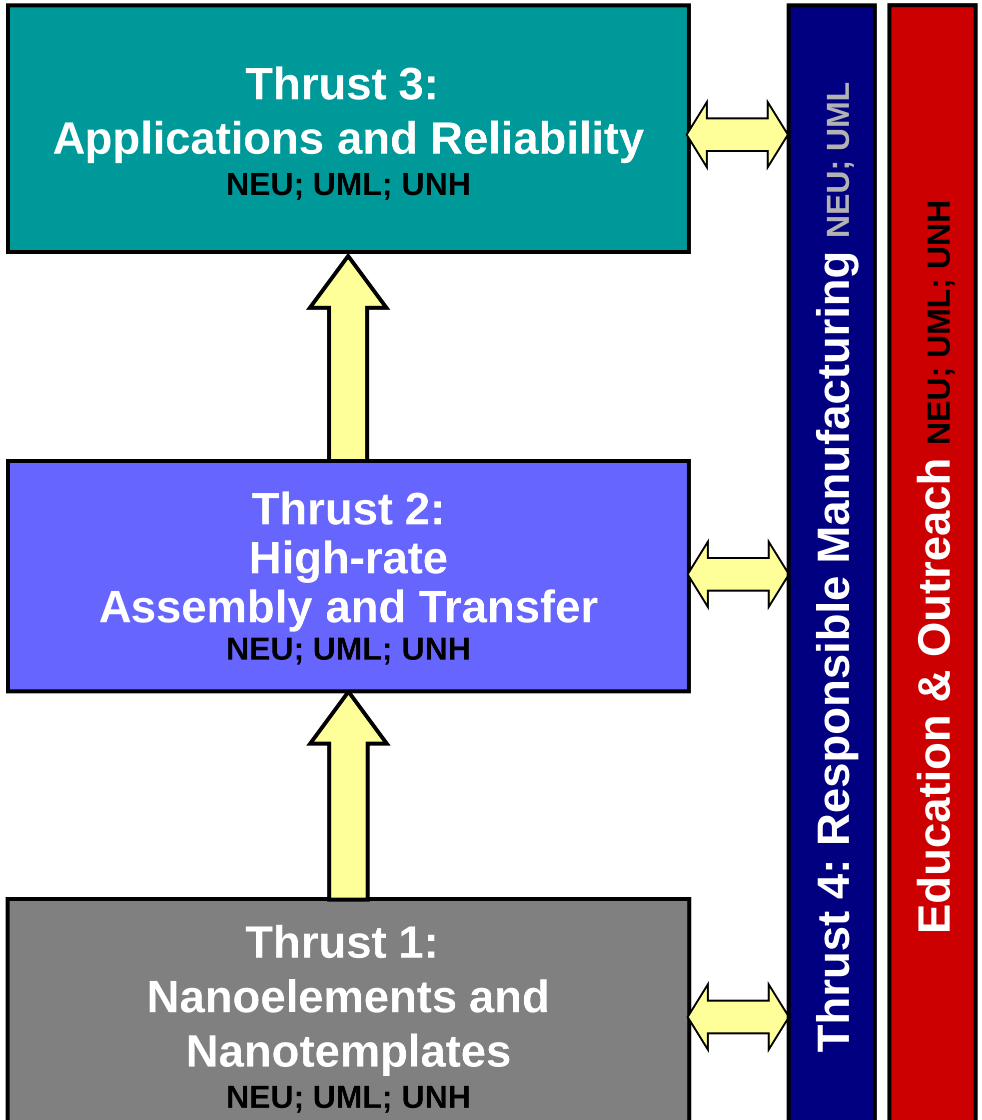
June 22-24, 2010

Northeastern University Research Team

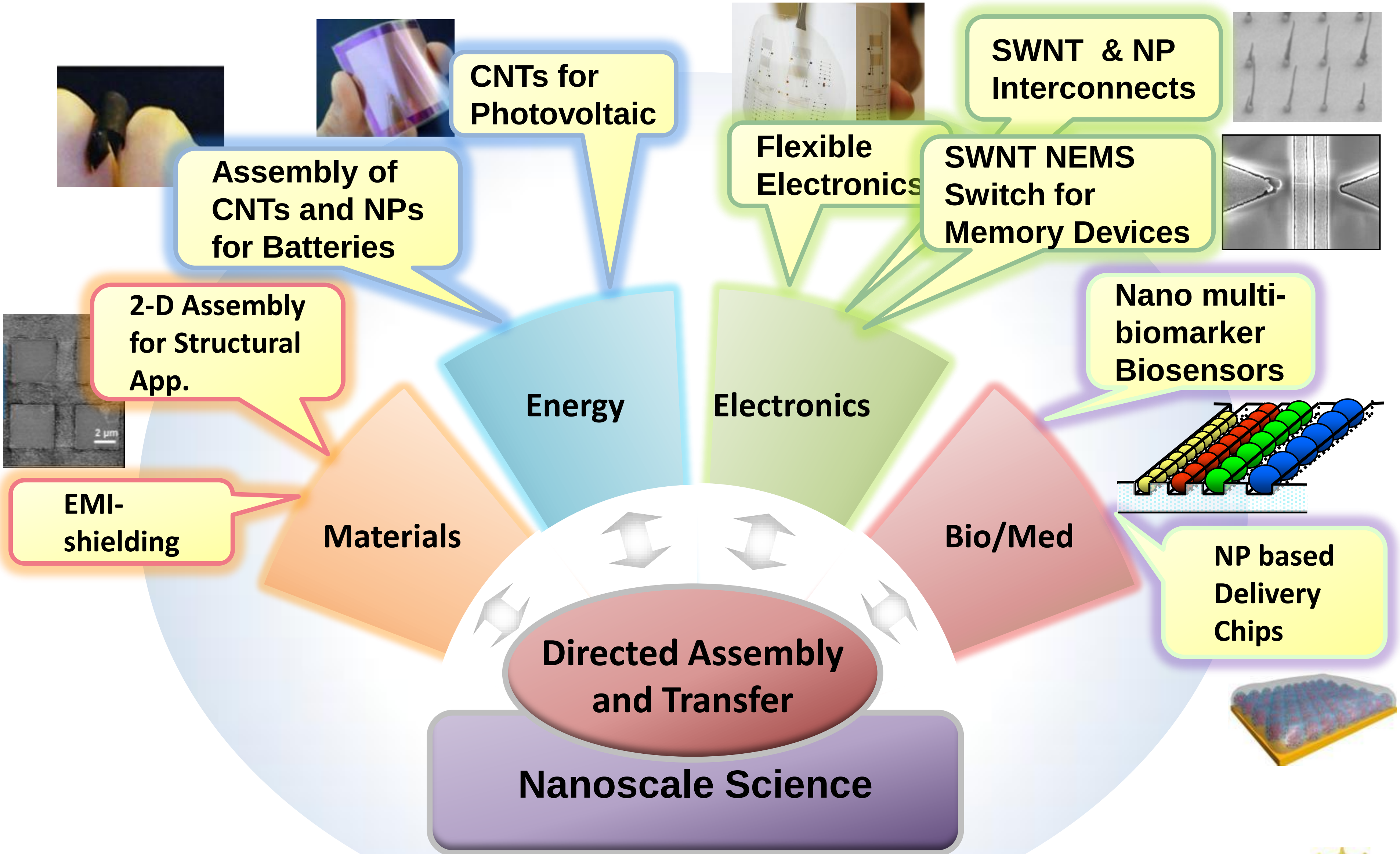
- Professor Jim Benneyan, Industrial Engineering (IE)
- Professor Chris Bosso, Political Science
- Lindsay Dahlben, M.S., Raytheon
- Zeynep Ok, Research Assistant, Ph.D. August 2010

- Serkan Erbis and Ali Hakimian, Graduate Research Assistants
- Angela Mongelluzzo, Zachary Roberts, Vanessa Porte, REUs

CHN Path to Nanomanufacturing

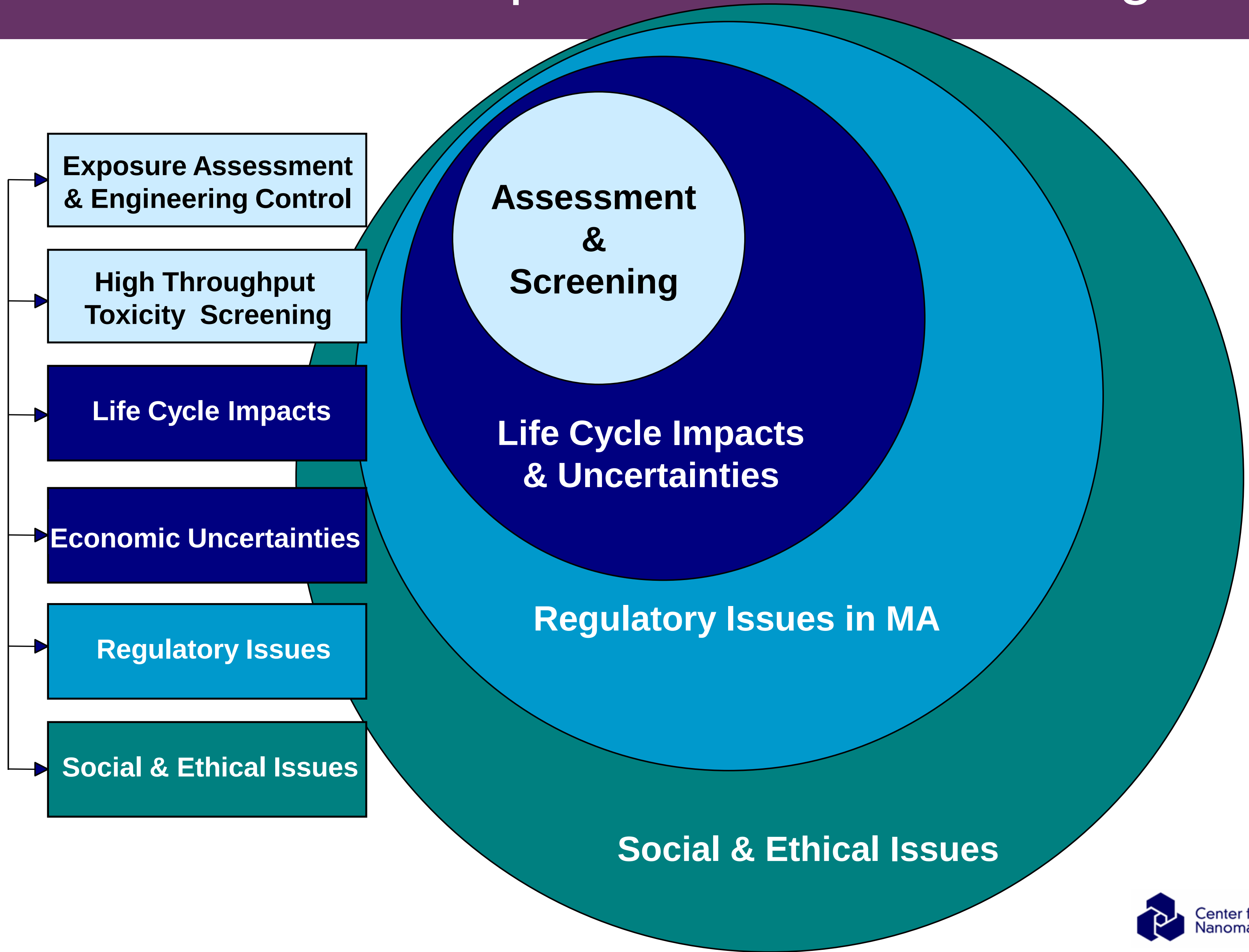


NSF Center for High-rate Nanomanufacturing Applications Road Map



Northeastern University | UMASS LOWELL | University of New Hampshire | Michigan State University | Museum of Science | NSF

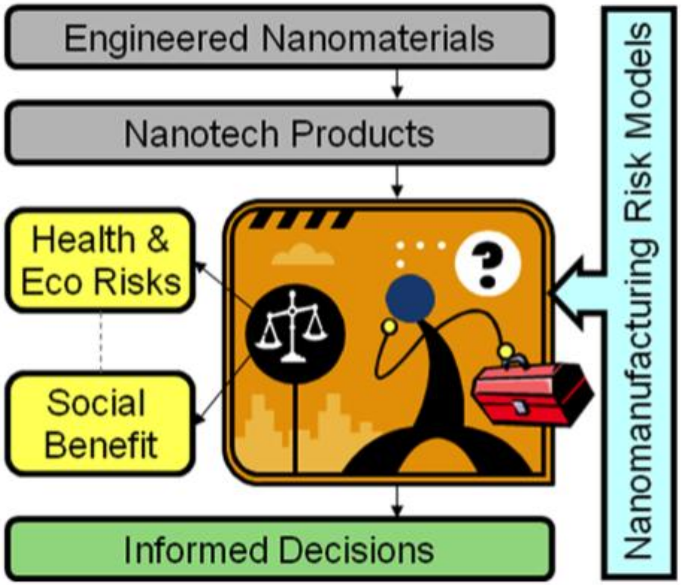
CHN Thrust 4: Responsible Manufacturing



Center for High-rate Nanomanufacturing

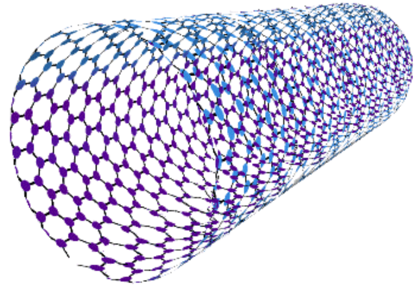
Nanomanufacturing promise and perils

- Enormous promise of nanotechnology in energy, medicine, electronics, consumer products, and other applications
- Uncertainty exists in:
  - Future market demand
  - Full-scale production economics
  - Environmental, health and safety (EHS) risks of nanomaterials
  - Appropriate workplace safeguards
  - Commercialization regulations
  - Environmental protections



Use of Modeling Tools to Reduce Uncertainty

Carbon Nanotubes

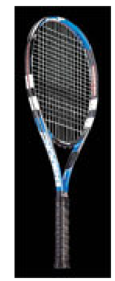


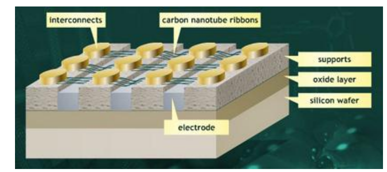
Properties

- High tensile strength, high Young's modulus, good thermal conductivity, metallic/semiconducting

CNT Global Market

- 2008: $90.5 million
- 2015: $1.44 billion





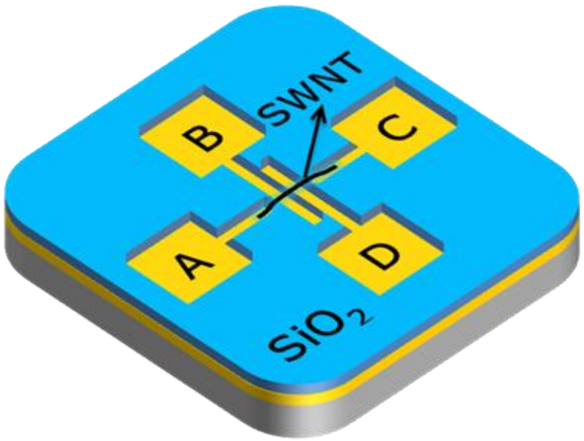
www.nanotechproject.org

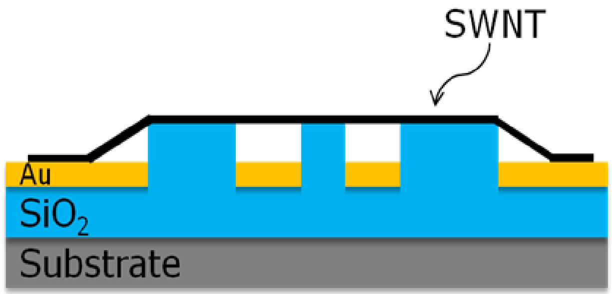
Human Health and Environment Issues

- Unique compared to bulk heterogeneous carbon
- Effects similar to asbestos (Poland et al. 2008), may cause inflammation, fibrosis (Shvedova et al. 2008)
- Lack of biodegradability (Helland et al. 2007), respiratory and neuro-toxic effects on trout (Smith et al. 2007)

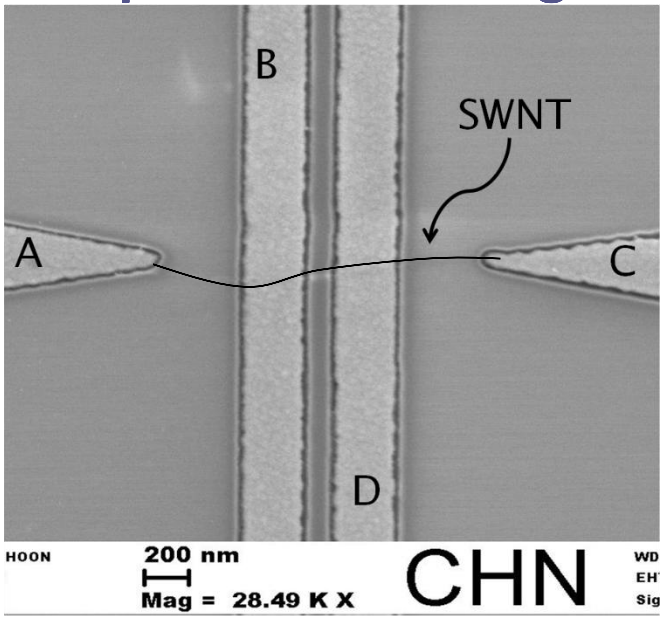
Case Study 1: CNT Switch

Isometric and cross-section schematics



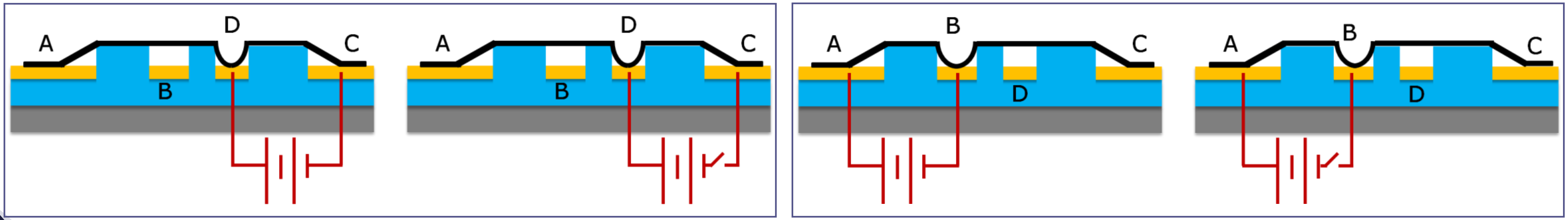


Top view SEM image



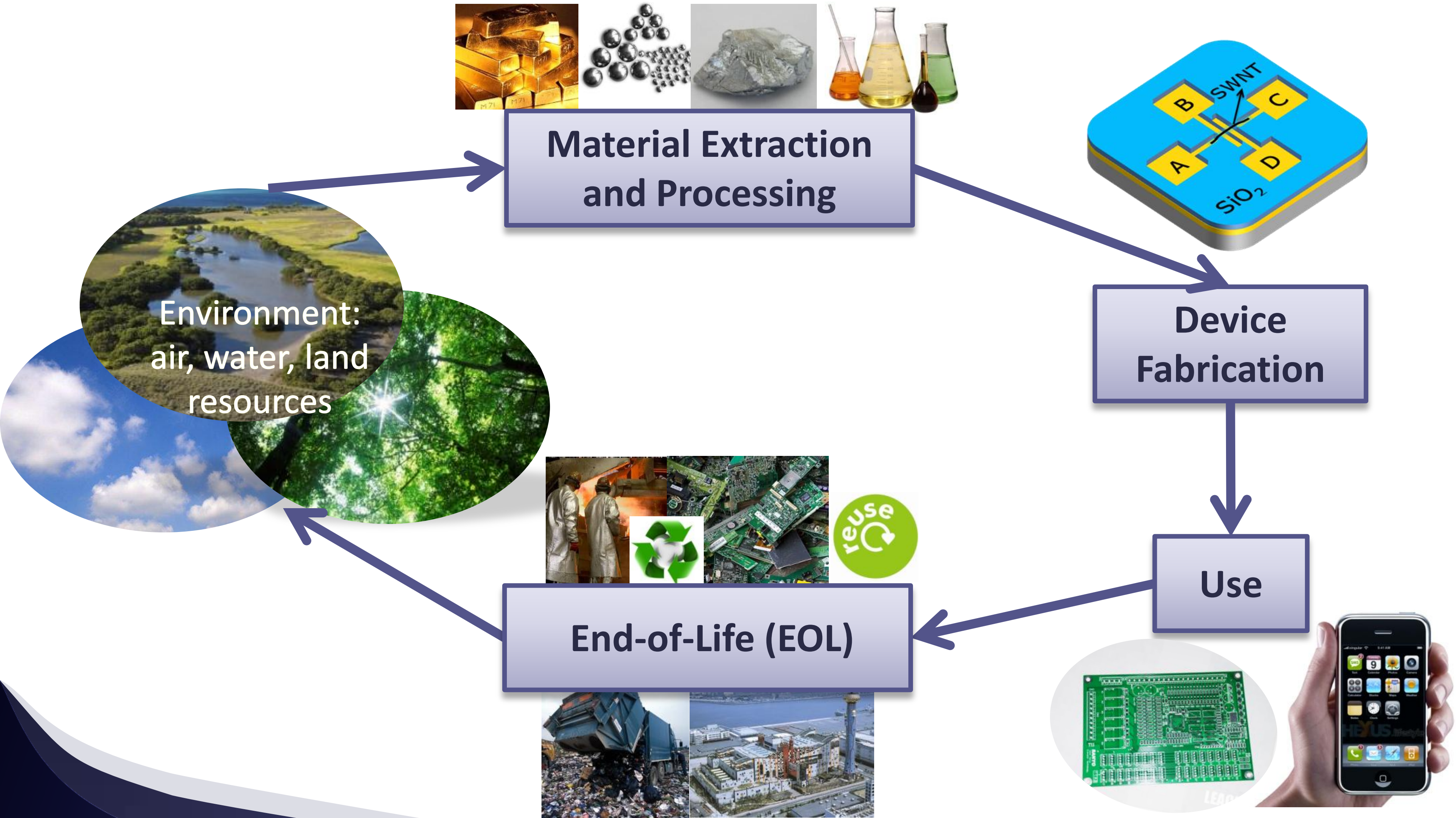
Properties

- High speed programming
- Low-voltage
- Resistance to temp., vibration



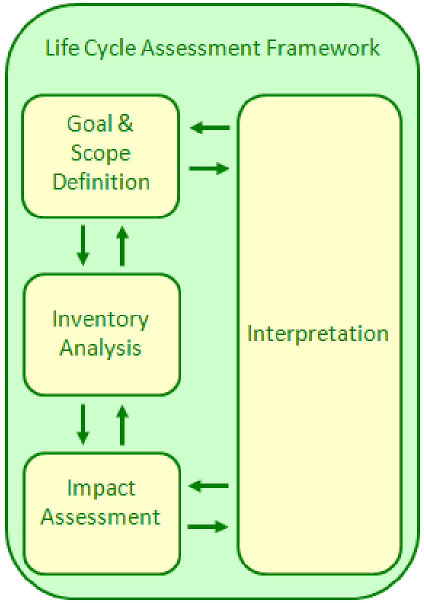
Principles of operation and non-volatility

CNT Switch Life Cycle



Methodology: LCA

- Life cycle assessment (LCA)
  - **Scope**: Up to fabrication, then extended to use and end-of-life
  - **Functional unit**: One 3” Si wafer
  - **Inventory** data gathered at CHN labs
    - Equipment, energy, process recipes, materials, total cycle times
    - Lab and full-scale fabrication environments
    - Wafer capacities, material reuse, yields
  - **Impact assessment** carried out using SimaPro™
    - Ecoinvent™ inventory database
    - Eco-indicator 1999™ impact assessment method



ISO 2006

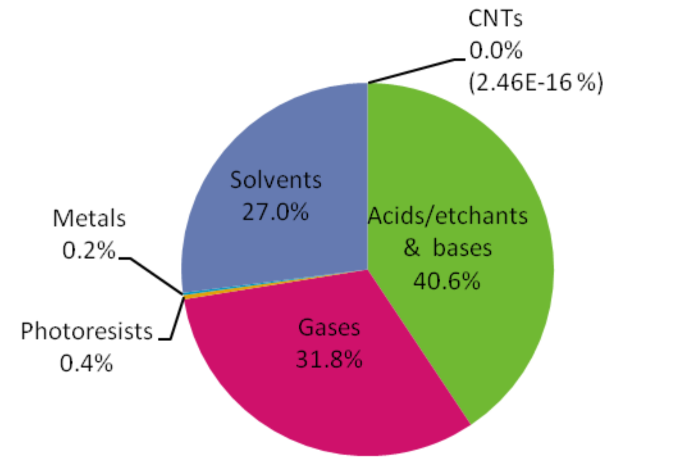
Fabrication Steps

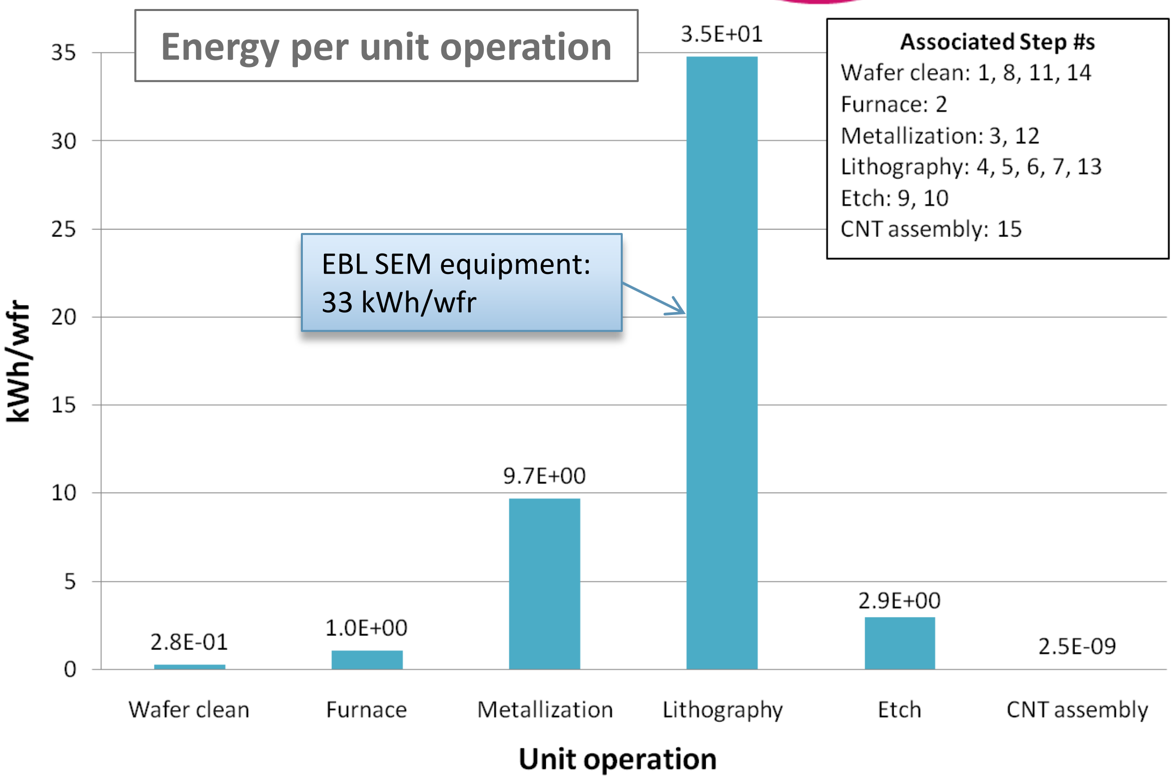
Step #	Unit operation	Function	Recipe
1	Wafer clean	Particulate removal	Standard pre-diffusion clean
2	Furnace	Film deposition	500 nm SiO_2 wet oxidation
3	Metallization	Film deposition	20 nm W sputter
4	Lithography	Resist coat	150 nm PMMA spin coat
5	Lithography	Resist bake	Oven bake
6 (Lab)	Lithography	Film patterning	EBL switch template
6 (Full)	Lithography	Film patterning	Optical switch mask alignment
7	Lithography	Resist development	MIBK/IPA solution
8	Wafer clean	Rinse and dry	Cascade rinse and dry
9	Etch	Film patterning	SF_6, CHF_3 plasma etch
10	Etch	Resist removal	HF wet etch
11	Wafer clean	Rinse and dry	Cascade rinse and dry
12	Metallization	Film deposition	2 nm Cr, 50 nm Au e-beam evaporation
13	Lithography	Film patterning	Lift-off
14	Wafer clean	Rinse and dry	Cascade rinse and dry
15	CNT assembly	CNT deposition	Dielectrophoresis

Lab-scale Fabrication Results

Energy and categorized input materials

ENERGY	
	[kWh/wfr]
	48.74
INPUT MATERIAL	
	[kg/wfr]
Acids/etchants & bases	0.2772
Gases	0.2169
Photoresists	0.0025
Metals	0.00142
Solvents	0.1841
Water	10.414
CNTs	1.68E-18
INPUT TOTAL (w/o water)	**0.68**
INPUT TOTAL (w/ water)	**11.10**





Scaled-up Fabrication Results

Input [kg/wfr]

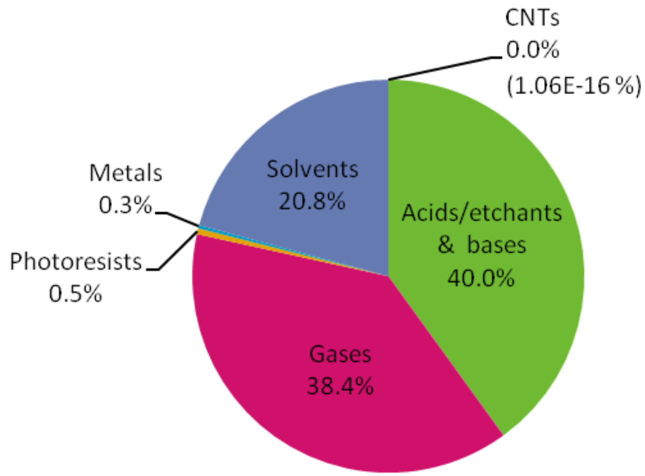
Acids/etchants & bases:	0. 213
Gases:	0.205
Photoresists:	0.0026
Metals:	0.0015
Solvents:	0.111
CNTs:	5.7E-19
Water:	678.5
Energy [kWh/wfr]:	0.0131

Full-scale wafer fabrication

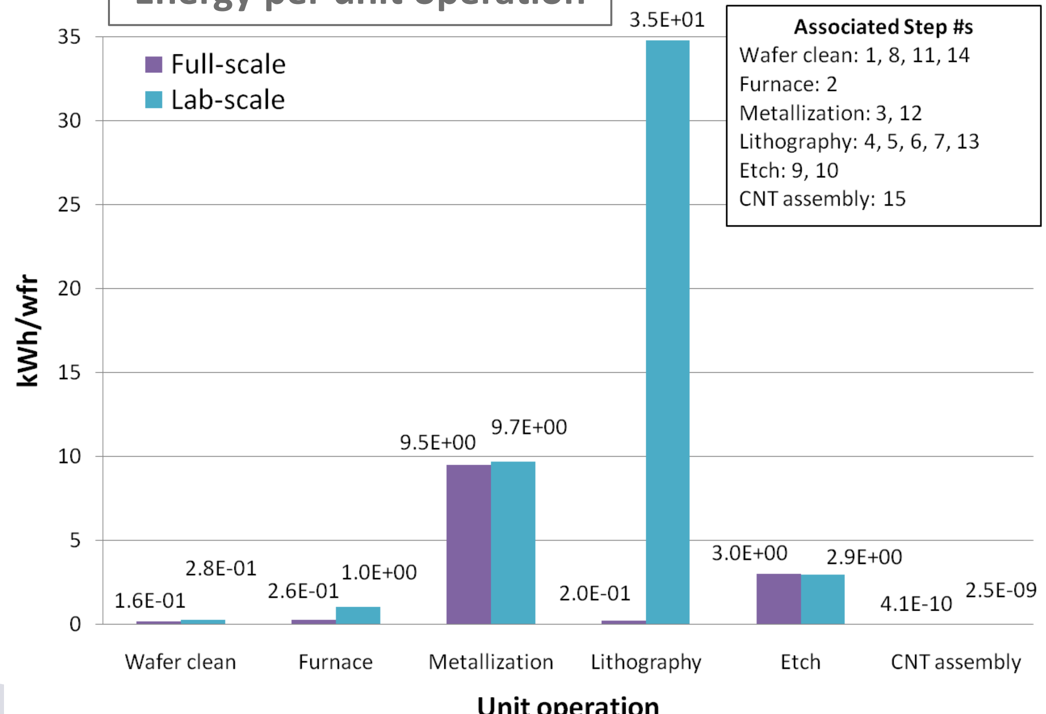
Output [kg/wfr]

Mixed wastewater to treatment:	701.0
Hazardous waste:	0.0975
Air emissions:	0.1996
CNTs:	5.7E-19

Input material (excluding water)



Energy per unit operation

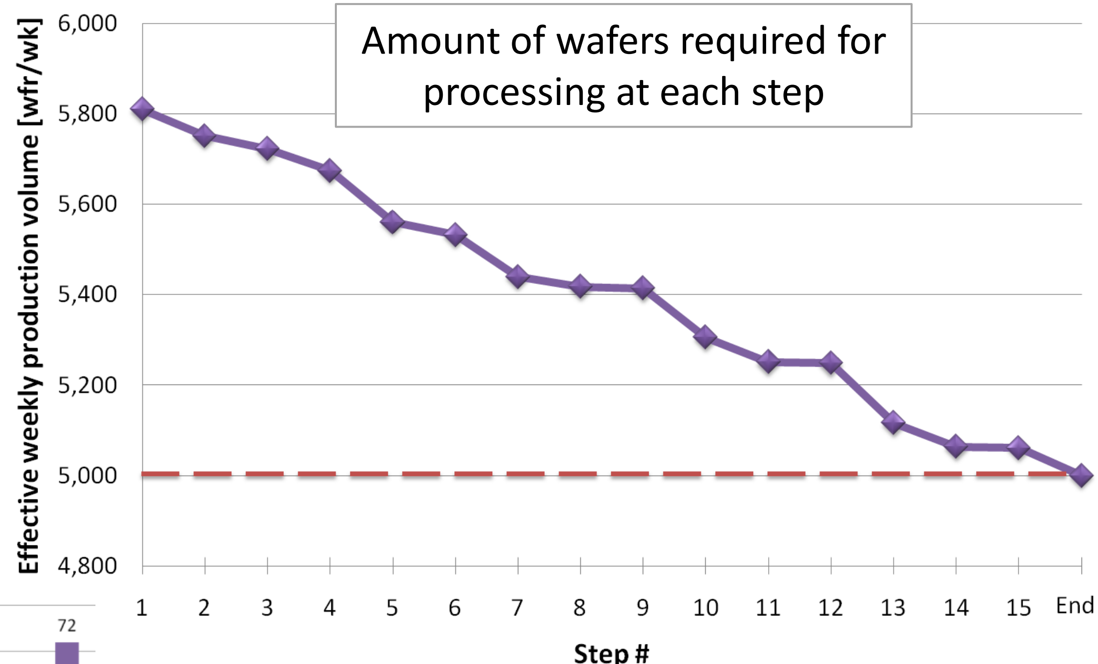


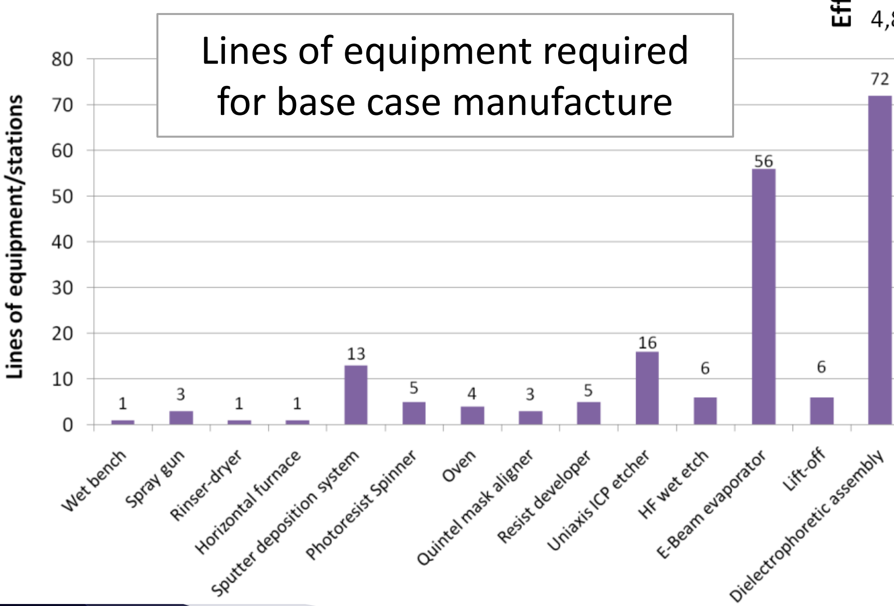
Calculations for Fab Scale-up

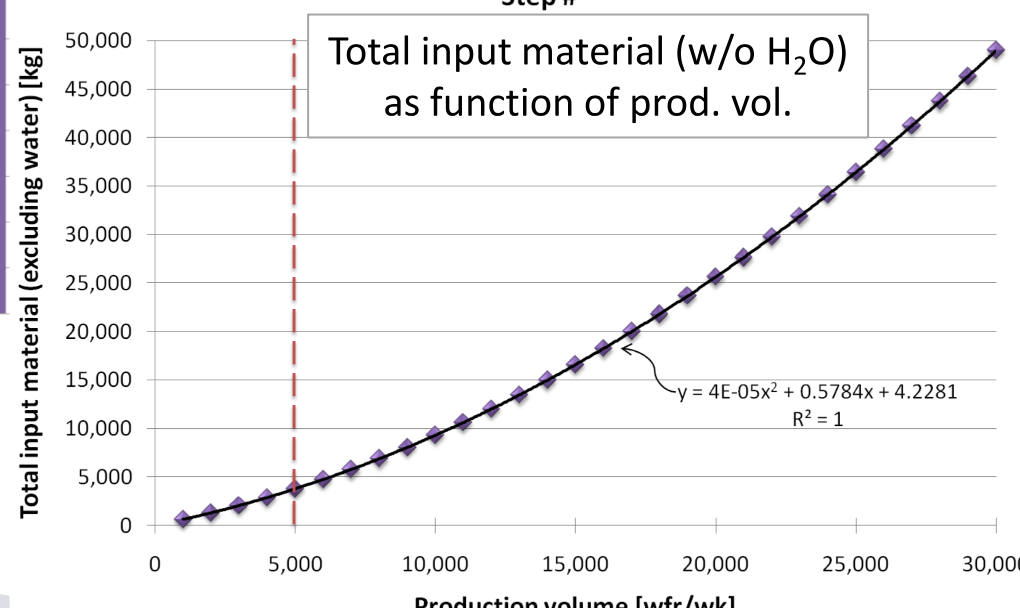
Base case manufacturing specifications

Weekly production volume	5,000 wfr/wk
Working hours per day	24 h/day
Working days per week	7 day/wk
Production time ("up-time")	80%
Production hours per week	134 h/wk

From Murphy 2003

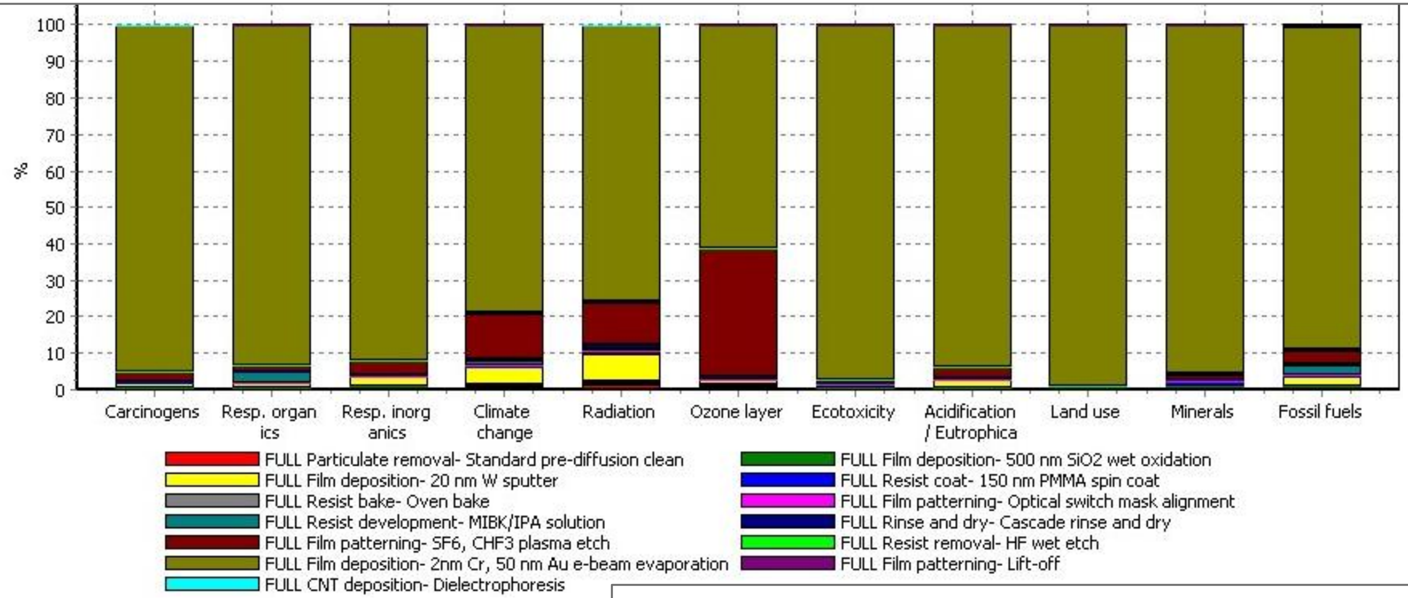






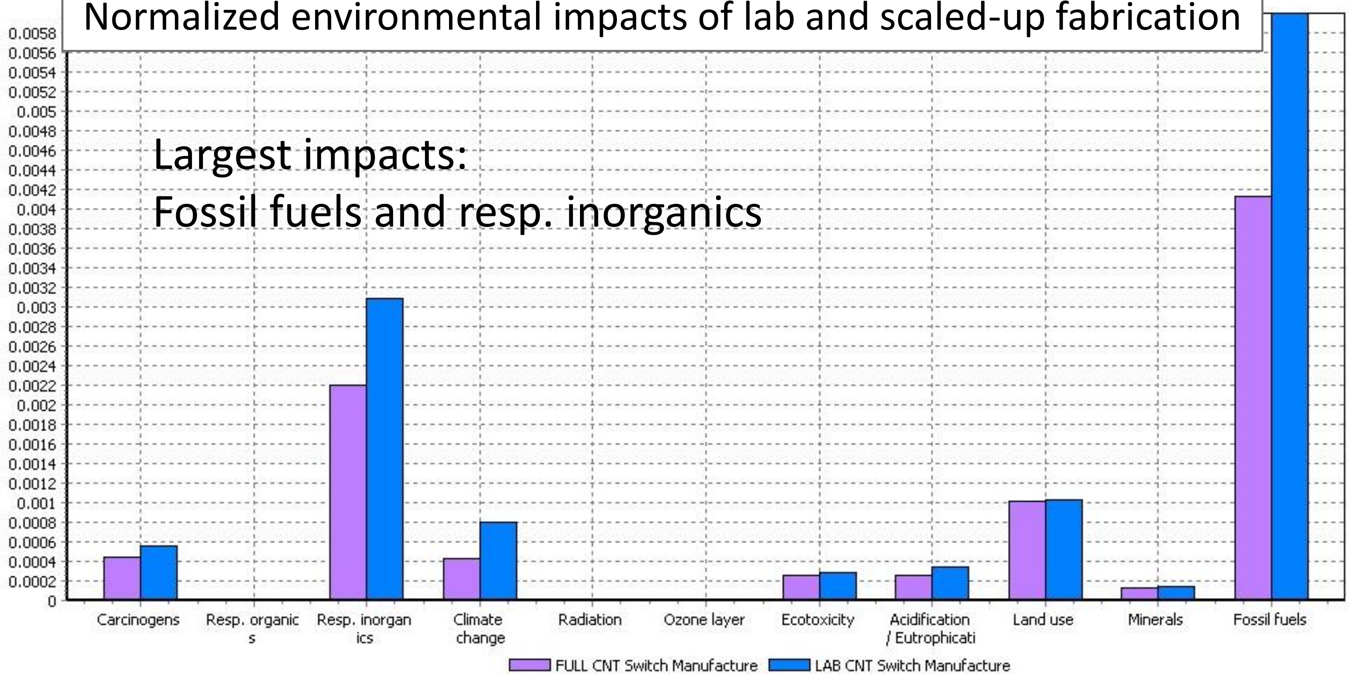
Impact Assessment Results

Characterization of environmental impact of full-scale CNT switch fabrication per wafer



Large impact due to use of gold deposition

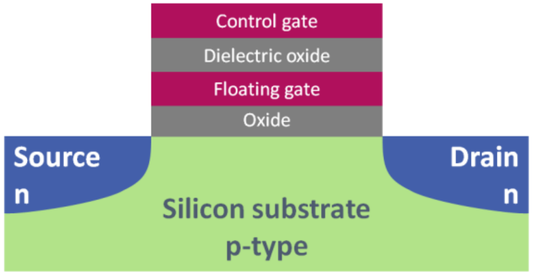
Normalized environmental impacts of lab and scaled-up fabrication



Largest impacts:
Fossil fuels and resp. inorganics

Use Stage

- CNT switch as replacement to existing FGMOSFETs in NAND flash memory
- 16 GB memory for cell phone application



Floating gate metal-oxide-semiconductor field-effect transistor (FGMOSFET)

Cell size = CF x F^2	NAND flash	CNT switch
Feature size (*F*) [nm]	40	180
Cell factor (*CF*)	4	12
Storage density [Gb/in^2]	62.9	1.5

Cell size = CF x F^2

6.4E-11 cm^2

vs.

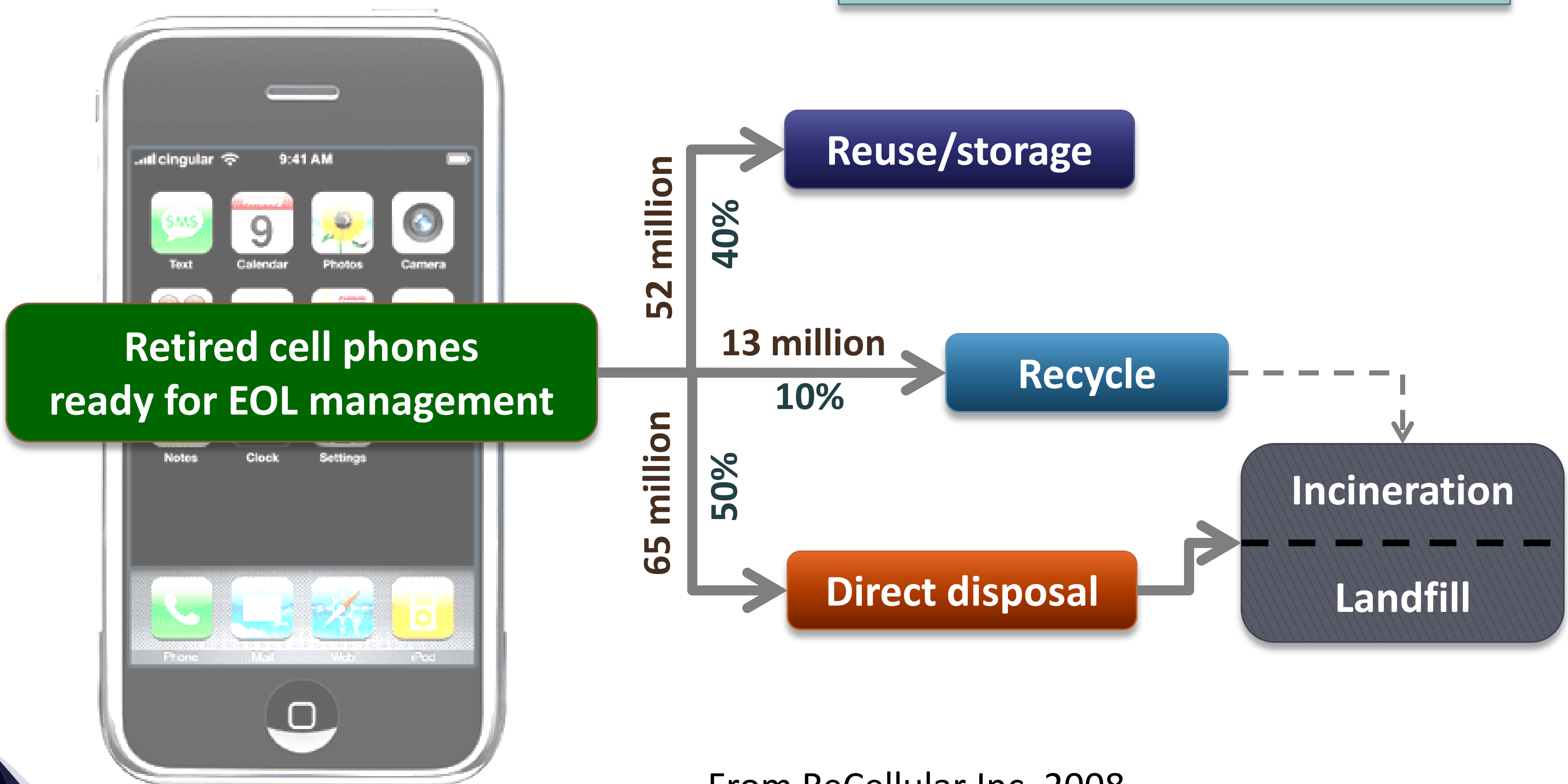
3.9E-9 cm^2

220 billion NAND flash cells vs. 153 billion CNT switch cells **30% less cells**

	Power [µW]			Speed of operation [ns]		
	NAND flash	CNT switch	% of NAND	NAND flash	CNT switch	% of NAND
Read	3.3E3	1.5E-1	0.005%	3.0E4	1.0E1	0.033%
Write	2.0E0	4.5E-1	22.5%	2.0E5	1.0E1	0.005%
Erase	3.3E0	1.5E-1	4.545%	2.0E6	1.0E1	0.001%
Cycle	6.61E3	9.0E-1	0.014%	2.26E6	4.0E1	0.002%

EOL Stage

Every year, 130 million cell phones are retired in the U.S.



From ReCellular Inc. 2008

Recycling Processes

- Mechanical and electromagnetic separation
  - Separate materials of different types, densities, sizes, magnetic properties
  - Includes shredding and crushing in hammer mills, eddy current, electrostatic separation
  - Not likely to eliminate CNTs during processing
  - Filtration systems may not be able to control CNT dispersion into air
- Extractive metallurgy
  - Thermal treatment and aqueous chemistry for metal recovery
  - Includes reduction, smelting, incineration
  - May oxidize and burn off CNTs if they become free-standing and the process temperature is high enough

Direct Disposal to Landfill & Incineration

How many CNTs could end up in landfills or be incinerated?

	Lower bound	Upper bound
Number of retired cell phones that contain CNT switch technology	20%	80%
EOL management options		
Reuse/storage	50%	20%
Recycle	15%	5%
Direct disposal—Landfill	20%	45%
Direct disposal—Incineration	15%	30%

First-order approximation

	Mass of CNTs [g]	
	Lower bound	Upper bound
Landfill	3.2	28.6
Incineration	2.4	19.1
Total to direct disposal	**5.6**	**47.7**

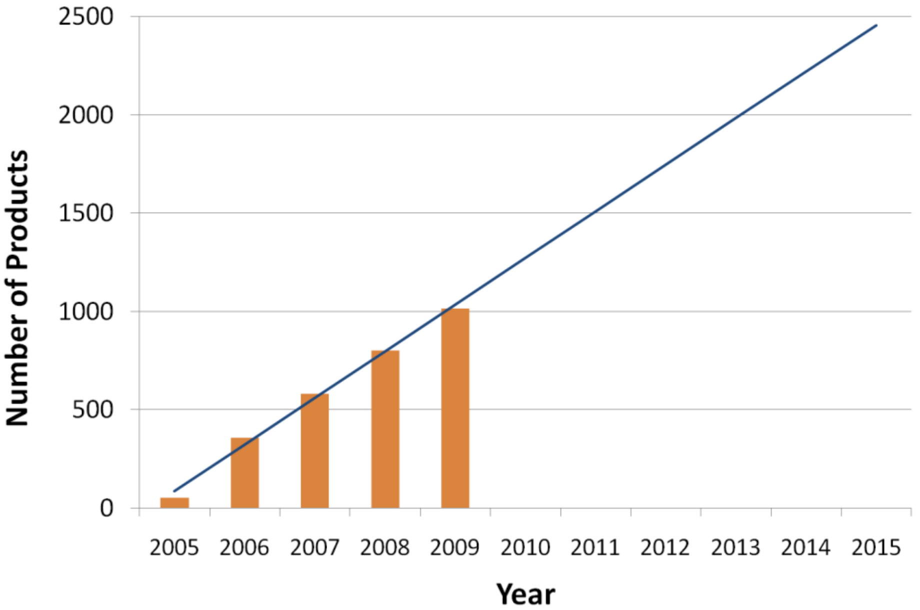
NOTE: Estimation is based on mass—other metrics (surface area, reactivity, persistence) may be better indicators for nanomaterials

Summary for LCA Case Study 1

- CNT switch investigated through life cycle to provide first-order depiction of environmental footprint
  - **Fabrication** resource use, predominantly energy, DI H_2O
  - **Full-scale** resource consumption lower than lab-scale
  - **Gold refining** greatest contribution to environmental impact
  - **Performance advantages** in use stage
  - **EOL** recycling issues identified and mass of CNTs calculated
- Continued inventory collection for other applications
  - Biosensor
  - Chemical sensor
  - Battery
- Development of Cost Models to predict mfg economics
- Alternatives assessment…

+ Rapid Market Growth and Commercialization

- **State of Nano-Market**
  - 1997: Zyvex – First company to research nanotechnology founded
  - 2007: $147 billion worth of nanotechnology-based products
  - 2015: Projected $3.1 trillion in global market



Total number of nanotechnology-based products listed in Consumer Product Inventory, with regression analysis

Little guidance regarding how to best manage nanotechnology workplace, development and commercialization decisions

Case Study 2: Nanomanufacturing Scale-up

Model inputs

Rapidly growing CNT mfger selecting among alternate facility expansion plans:

	Space (square foot)	Expansion Capability (% increase)	Operating Cost ($/time)	Throughput (amount/time)	Safety (level)	Safety Uncertainty (level)
Design 1	30,000	300	700,000	850	5	1-10
Design 2	30,000	600	700,000	1,700	8	5-10
Design 3	30,000	900	700,000	2,550	10	8-10
Design 4	80,000	700	1,120,000	2,150	5	1-10
Design 5	80,000	1400	1,120,000	4,300	8	5-10
Design 6	80,000	2100	1,120,000	6,500	10	8-10

Discrete, multi-criteria optimization

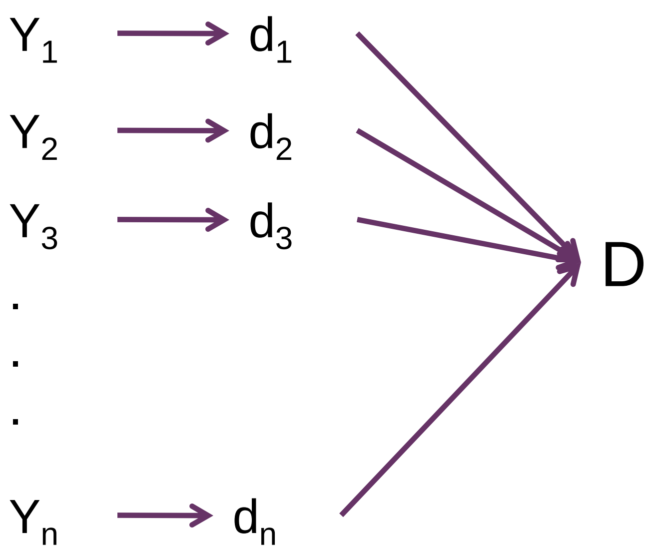
Methodology: Desirability Functions

Identified **desirability optimization** as one of the most promising decision support tools for assessing and managing nanomanufacturing development decisions

- Each criteria Y_i transformed to a dimensionless value d_i
- d_i increases as the desirability of Y_i increases
  - $0 \leq d_i \leq 1$
  - $d_i = 0.00$ completely undesirable
  - $d_i = 1.00$ completely desirable or ideal
- Individual d_i values combined into an overall desirability index, D

Desirability Approach

Framework for
- Choosing between finite number of alternatives
- Identify optimal process variable settings



1. Define individual desirability functions for each criteria
2. Transform each criteria's value, Y_i, to a desirability value, d_i
3. Combine individual d_i values into overall desirability index, D
4. Solve the multi-criteria optimization model to find the optimum solution that maximizes D

Overall Desirability Index, *D*

- Geometric mean

$$D = (d_1 d_2 d_3 \dots d_n)^{1/n}$$

- Weighted geometric mean

$$D = \left(d_1^{w_1} d_2^{w_2} d_3^{w_3} \dots d_n^{w_n}\right)^{1/\sum w_i}$$

- Minimization operator

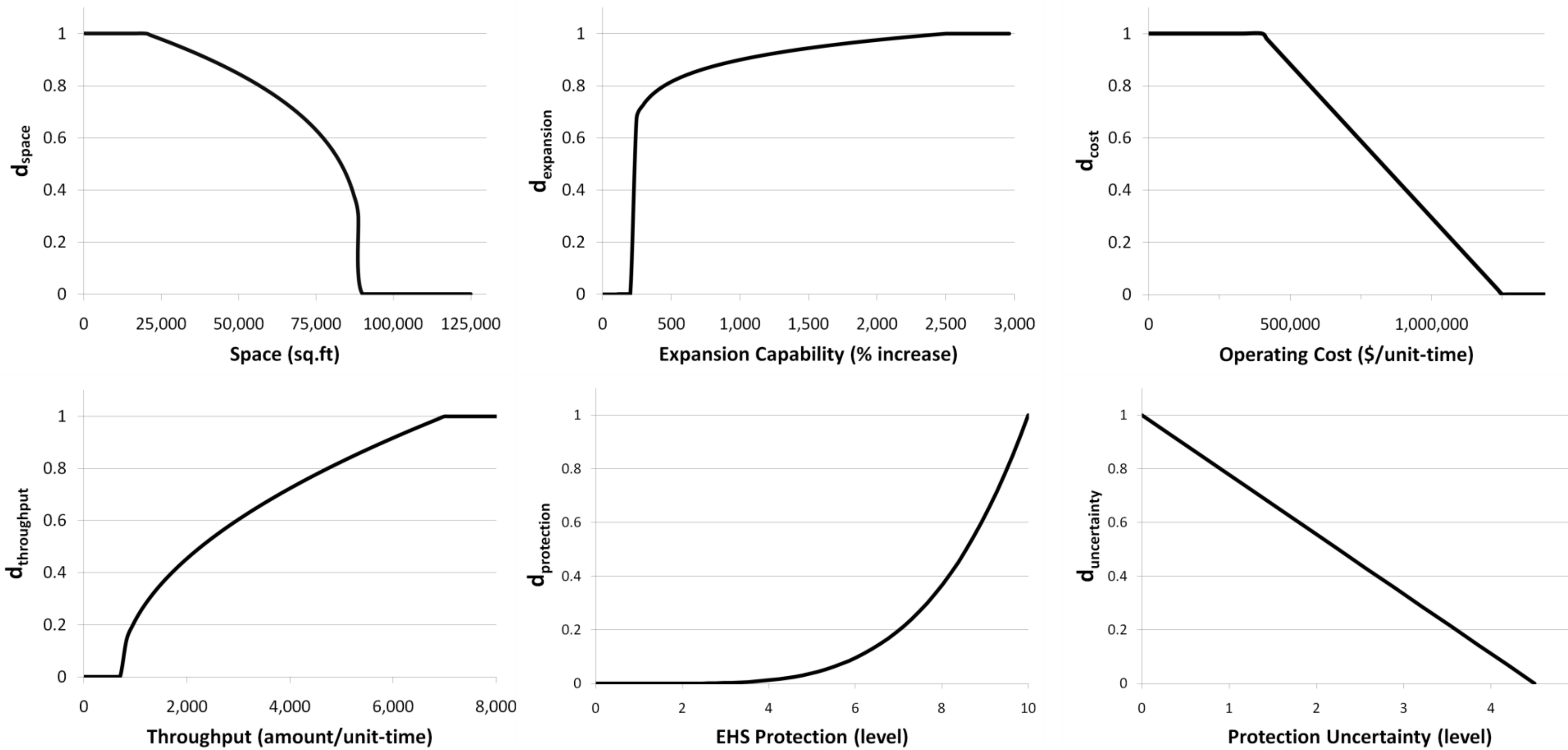
$$D = min(d_1, d_2, d_3, \dots, d_n)$$

These methods ensure that:

- *D* will fall in the interval [0,1] and
- If any $d_i = 0$, then overall desirability is unacceptable ($D = 0$).

Desirability Functions Defined…

Facility design desirability functions for space, expansion capability, operating cost, throughput, EHS protection, and protection uncertainty



Desirability Optimization

$$D = \left(d_1^{w_1} d_2^{w_2} d_3^{w_3} \dots d_n^{w_n}\right)^{1/\sum w_i}$$

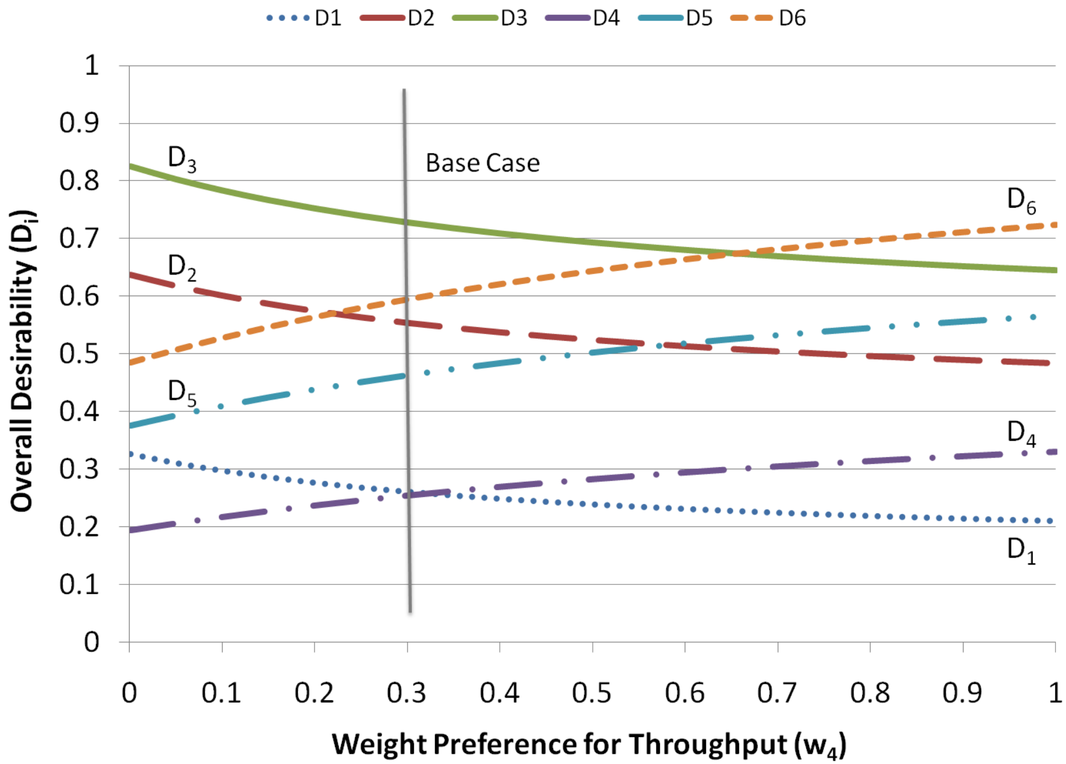
	Space	Expansion Capability	Operating Cost	Throughput	Safety	Safety Uncertainty	Overall Desirability
Design 1	30,000	300	700,000	850	5	1-10	0.26
Design 2	30,000	600	700,000	1,700	8	5-10	0.55
Design 3	30,000	900	700,000	2,550	10	8-10	0.73
Design 4	80,000	700	1,120,000	2,150	5	1-10	0.25
Design 5	80,000	1400	1,120,000	4,300	8	5-10	0.46
Design 6	80,000	2100	1,120,000	6,500	10	8-10	0.60

Largest D: The most desirable design alternative (best selection) in terms of balancing all decision criteria

+ Sensitivity Analysis

w_i (Criteria)	Optimal Solution: Design 3	Optimal Solution: Design 6
w_1 (Space)	$0 < w_1 \le 1$	
w_2 (Expansion)	$0 < w_2 \le 1$	
w_3 (Cost)	$0.1 < w_3 \le 1$	$0 < w_3 \le 0.1$
w_4 (Throughput)	$0 < w_4 \le 0.65$	$0.65 < w_4 \le 1$
w_5 (EHS Protection)	$0 < w_5 \le 1$	
w_6 (Uncertainty)	$0 < w_6 \le 1$	

Base Case:
$w_1 = 0.05$, $w_2 = 0.15$,
$w_3 = 0.25$, $w_4 = 0.30$,
$w_5 = 0.15$, and $w_6 = 0.10$

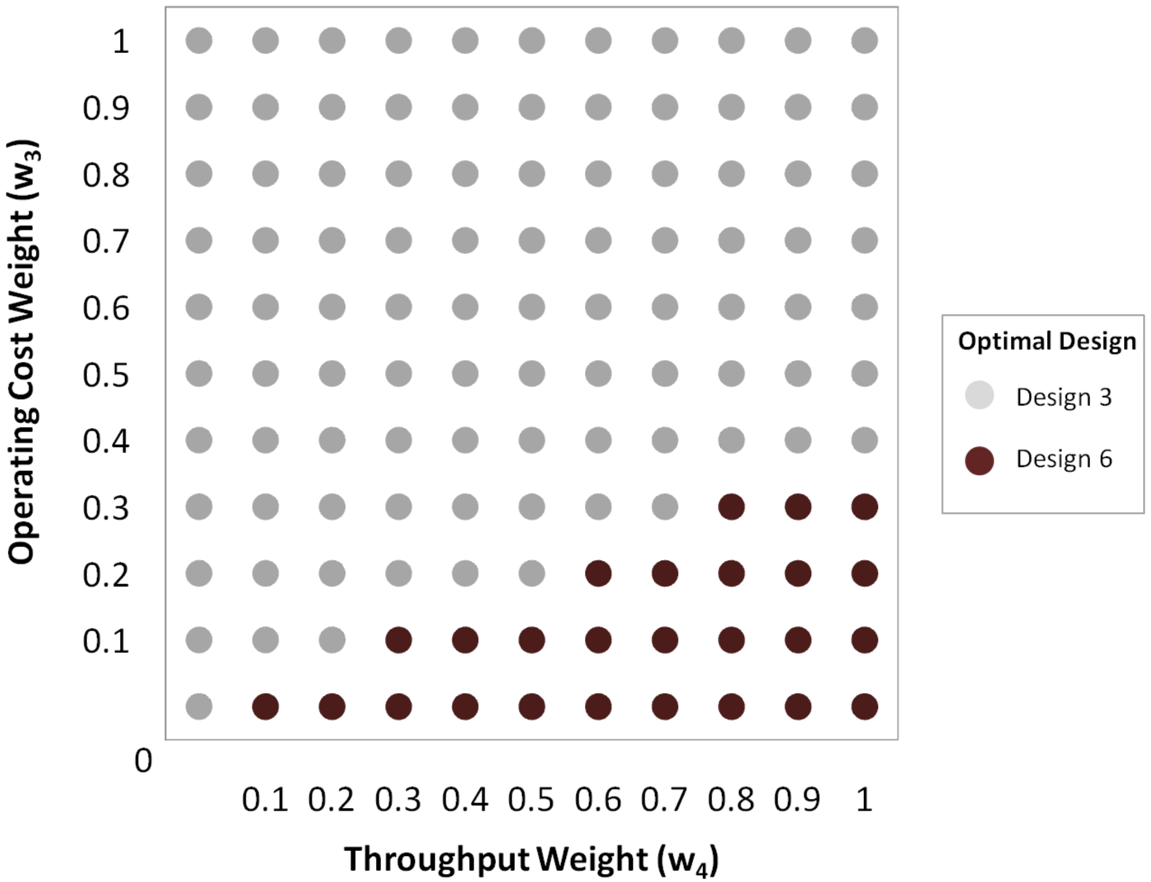


Sensitivity of overall desirability indices, D, of six alternate designs to increasing or decreasing the weight preference for throughput

Optimal Design Determined

Illustration of optimal designs for various combinations of operating cost and throughput weights

Robust model



Summary for Case Study 2

- Managing trade-offs among nanomanufacturing safety, production, and cost in a ‘safe’ facility design is both difficult and important
- Sensitivity and what-if analyses on the results provide useful insights for better management of uncertainties
- Models can help decision-makers develop a more informed understanding of trade-offs regarding nanotechnology manufacturing and commercialization

Modeling Tools Can Aid in Identification of Uncertainties

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Northeastern University

Center for High-rate Nanomanufacturing

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NSF

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